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X-652-73-261
PREPRINT

NASA TM X-70466

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(NASA-TM-X-70466) RESEARCH NEEDS IN OCEAN COLOR DATA ANALYSIS (NASA) 17 p HC $3.00 CSCL 08J

N73-31355

Unclas
G3/13 14059



SEPTEMBER 1973

GSFC

GODDARD SPACE FLIGHT CENTER
GREENBELT, MARYLAND

X-652-73-261

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September 1973

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## ABSTRACT

The success of the effort to extract several subsurface oceanographic parameters from remotely sensed ocean color data will depend to a great extent upon the existence of adequate theoretical models relating the desired oceanographic parameters to the upwelling radiances to be observed. In order to guide the development of these models, and to check their accuracies, a considerable amount of experimental work must be performed. The theoretical and experimental work which will be needed to develop techniques for the quantitative analysis of satellite ocean color data is described.

CONTENTS

## RESEARCH NEEDS IN OCEAN COLOR DATA ANALYSIS

### INTRODUCTION

A large number of techniques have been developed for sampling the ocean from top to bottom. Vertical profiles of most of the major chemical, physical, and biological parameters abound in the literature. But horizontal sampling of the ocean has been conducted on a reasonable scale only rarely, and then only at considerable expense of time and money. It is true that a suitably equipped research vessel can cover large areas of the ocean and collect a large amount of data, in a single cruise. However, with relatively small cruising speeds the extent of possible simultaneity of the measurements is severely limited.

As the field of oceanography becomes more and more sophisticated, with many scientists actively involved in large-scale or even global modeling of oceanographic parameters, the unavailability of global synoptic data is becoming a critical deficiency. Until the number of available suitably equipped research vessels increases several orders of magnitude and their maximum speeds increase very substantially, neither of which are very likely to happen in the near future, we shall be forced to rely on data collected by aircraft and satellites in order to obtain the kind of large-scale synoptic data that is needed to build accurate global models suitable for prediction. The need for global synoptic data on the oceans is so great that much effort will be expended in this decade aimed at obtaining this data by remote sensing, both actively and passively from aircraft and satellites.

Until the maximum weight and power limitations imposed on present-day scientific satellites is permitted to expand significantly, most of the data on the sea collected from spacecraft will necessarily be limited to the passive mode. Due to the essentially opaque nature of seawater outside the visible (and near ultra-violet) portion of the electromagnetic spectrum, passive remote measurements of subsurface oceanographic parameters will necessarily be limited to the visible portion of the spectrum. By "subsurface" we here mean the region from a few millimeters to a few tens of meters depth, the region of penetration of sunlight and skylight into the sea.

Although much work has been done in analyzing ocean color data gathered by a variety of sensors, including the multispectral scanner on ERTS-1, much of this analysis has been purely qualitative in nature. It is not yet clear which subsurface oceanographic parameters we can measure from space with the needed accuracy on a quantitative basis.

An experimental and theoretical effort is needed in order to determine these parameters and the measurement accuracies we can expect for each one. This

research effort will also be needed in order to develop the techniques of data analysis which will be needed in order to attain the predicted measurement accuracies. The description of such a research program is the purpose of this paper.

## PATTERN RECOGNITION APPLIED TO OCEAN COLOR DATA ANALYSIS

Due to weight, cost, and data transmission rate limitations, any mapping type remote sensor of ocean color must necessarily collect light from the sea in a finite number of channels. Data so obtained is particularly well-suited for analysis using the techniques of pattern recognition which have been extended for use with multispectral scanning remote sensors in the last few years. In this case, objects on the ground are identified, or recognized, by their spectral signatures rather than by their shapes. With this technique, a spectral signature is represented as an N-component vector whose components are the output signals of the N spectral channels of the remote sensor.

A spectral signature to be recognized is represented as a labelled point $\underline{a}$ in an N-dimensional vector space. By definition, if a given, but as yet unidentified, spectral signature vector $\underline{b}$ coincides with point $\underline{a}$ in the N-dimensional space then we say that $\underline{b}$ has been recognized (as $\underline{a}$). If it does not, then we say that $\underline{b}$ has not been recognized.

In practice, a parameter in the surface scene which is of interest (let's call it A) will have a large number of spectral signatures associated with it. In many cases, these will cluster in some identifiable region of the N-dimensional vector space and our test on the unknown spectral signature $\underline{b}$ will be whether its signature vector lies within the region of space which we have associated with surface parameter A. If it does, then we say that $\underline{b}$ has been recognized.

We shall call the regions of our N-dimensional space which are associated with corresponding surface parameters of interest <u>spectral recognition categories.</u> In general, the recognition problem is simplest when all the recognition categories associated with the surface features in which we are interested are well-defined and do not overlap. This is the case, for example, when we wish to distinguish the spectral signatures of a densely foliated forest and a freshly plowed field with a large number of channels equally spaced over the visible and near infrared portion of the spectrum. The recognition problem is difficult (and hence less accurate) when the recognition categories are not particularly well-defined and when they overlap.

It might be possible, in a few cases, to extend the concepts of spectral pattern recognition mentioned above, to the measurement of subsurface oceanographic parameters. In this case, instead of recognizing objects, such as red mangrove trees, by their spectral signatures, one would attempt to recognize a certain level,

say, of chlorophyl concentration by its spectral signature. But with the remote sensing of subsurface oceanographic parameters the associated spectral recognition categories are not likely to be well defined and they are likely to exhibit a considerable amount of overlap, even when the number N of spectral channels is large and their locations are carefully chosen so as to minimize this overlap.

The goal of any program aimed at developing techniques of analysis of remotely sensed ocean color data should be to develop techniques for accurately defining the spectral recognition categories associated with each of the subsurface oceanographic parameters of interest and to use this information to guide the choice of remote sensor spectral channels so as to minimize overlapping of the recognition categories associated with these oceanographic parameters.

It is felt that this can only be done through the development of a sizable surface truth experimental program used in conjunction with quantitative models of radiative transfer in the sea and in the atmosphere. Considerable effort has already gone into atmospheric models. An analogous program, both observational and theoretical, is needed for the sea.

## OPTICAL PROPERTIES OF THE SEA

Optically, the sea should be viewed as a polydisperse assembly of randomly oriented irregular particles which are capable of absorption, suspended in a locally homogeneous medium also capable of absorption.

The two major physical processes that affect the propagation of electromagnetic radiation in the sea are absorption and scattering. Scattering in the sea, as in the atmosphere, has two entirely different components. The first comes from molecular scattering by water and various salts and other substances dissolved in it. The second is due to scattering from particulates suspended in the water whose index of refraction is different from that of the surrounding medium.

In the open ocean and at scattering angles less than about $30^{o}$ (Mie) scattering by the suspended particles greatly predominates over (Rayleigh) molecular scattering. In the more turbid coastal regions, particulate scattering often predominates throughout the full angular range.

There are two general classes of particulates, the organic and the inorganic, which are distinguished by differences in their most abundant size ranges and differences in their indices of refraction relative to the medium. The organic particles have a very low index of refraction, in the range from 1.01 to 1.03 relative to sea water. The inorganic particulate index of refraction is closer to 1.15.

Scattering in the ocean is strongly dependent upon the angle of scattering, and both absorption and scattering, (by both molecules and particulates) are in general dependent upon wavelength.

Absorption within the particles has a great influence on the scattering properties of the medium over all visible wavelengths and must therefore be considered in any treatment of the scattering problem.

Since both absorption and scattering are capable of removing energy from a beam, it is impossible to measure absorption directly in any media or spectral regions where the scattering contributes significantly to the total loss of light from the beam. Extinction refers to the combined loss of energy from a beam by both absorption and scattering. Thus by measuring both extinction and total scattering, the absorption can be determined.

## REMOTE SENSING OF OCEAN COLOR

The upwelling radiance just below the sea surface is made up of sun and sky light which has been multiply scattered, with spectrally selective absorption and scattering by both the molecular and particulate components in the sea water contributing to the shape of the upwelling radiance spectrum. Thus, the wavelength spectrum of this upwelling light will depend upon the amount and kinds of dissolved substances in the water, and upon the amount and kinds of suspended particulates, both organic and inorganic.

Thus, it is in principle possible to determine a number of subsurface oceanographic parameters by measurements of the spectral distribution of radiant flux emerging from the sea. But there is a great variety of dissolved and particulate substances which are found in the world's oceans (especially in the coastal regions).

Due to this, the actual determination of oceanographic parameters from measurements of upwelling spectral radiances, will depend to a great extent upon the existence of adequate theoretical models relating the desired subsurface oceanographic parameters to the optical properties (absorption and scattering) of the water and then relating these properties to the observed upwelling radiances.

At present, very little of the needed modeling has been done. Thus, the major objective of the data analysis program which is described here should be the development of adequate models of the optical properties of all kinds of sea water, suitable for use with available atmospheric models, in order to relate satellite-observed spectral radiances to the desired oceanographic parameters in the sea.

Determination of the accuracy and validity of the model will depend upon extensive measurements of the absorption and scattering properties of sea as a function of wavelength and depth and simultaneous measurements of the up-and-down-welling spectral radiances at the sea surface. The performance of these measurements should be another major objective of the ocean color data analysis program.

## AN OPTICAL MODEL OF NATURAL WATERS

In order to properly interpret the data acquired by an ocean color multispectral sensor, one should have available a computerized theoretical model relating the subsurface oceanographic parameters of optical importance to the spectral distribution of upwelling radiance emerging from the sea surface and, through the use of an optical model of the atmosphere, the upwelling radiance emerging from the atmosphere. As mentioned before, considerable progress has already been made on the atmospheric model. Only the oceanic model remains.

The oceanic model can be conveniently divided into two separate stages, or components. See Figure 1. The first we shall call the microscopic model and the second the macroscopic model. The reason for this distinction will be made clear as the models are described in the next two sections.

In addition, an observational program is needed to evaluate the accuracy and validity of the models and to provide input data for the models. The measurements which need to be made can be conveniently divided into three separate categories. First are direct measurements of the subsurface oceanographic parameters of optical importance. Second are measurements of the optical properties (absorption and scattering) of the sea water. Third are measurements of the upwelling spectral radiances emerging from the sea which are to be detected by remote sensing equipment. Each of the above research categories will be discussed separately.

## THE MICROSCOPIC OPTICAL MODEL

The function of the microscopic optical model is to take the known concentrations of various substances dissolved and suspended as particles in sea water together with their known absorption and scattering properties in order to predict the bulk absorption and scattering properties of the medium. In general the molecular constituents are handled differently from the particulates. The spectral absorption coefficients of the molecular constituents can be obtained from published measurements where they exist, or they can be measured using commercially available instruments.

OPTICAL MODEL OF THE SEA FOR REMOTE SENSING APPLICATIONS

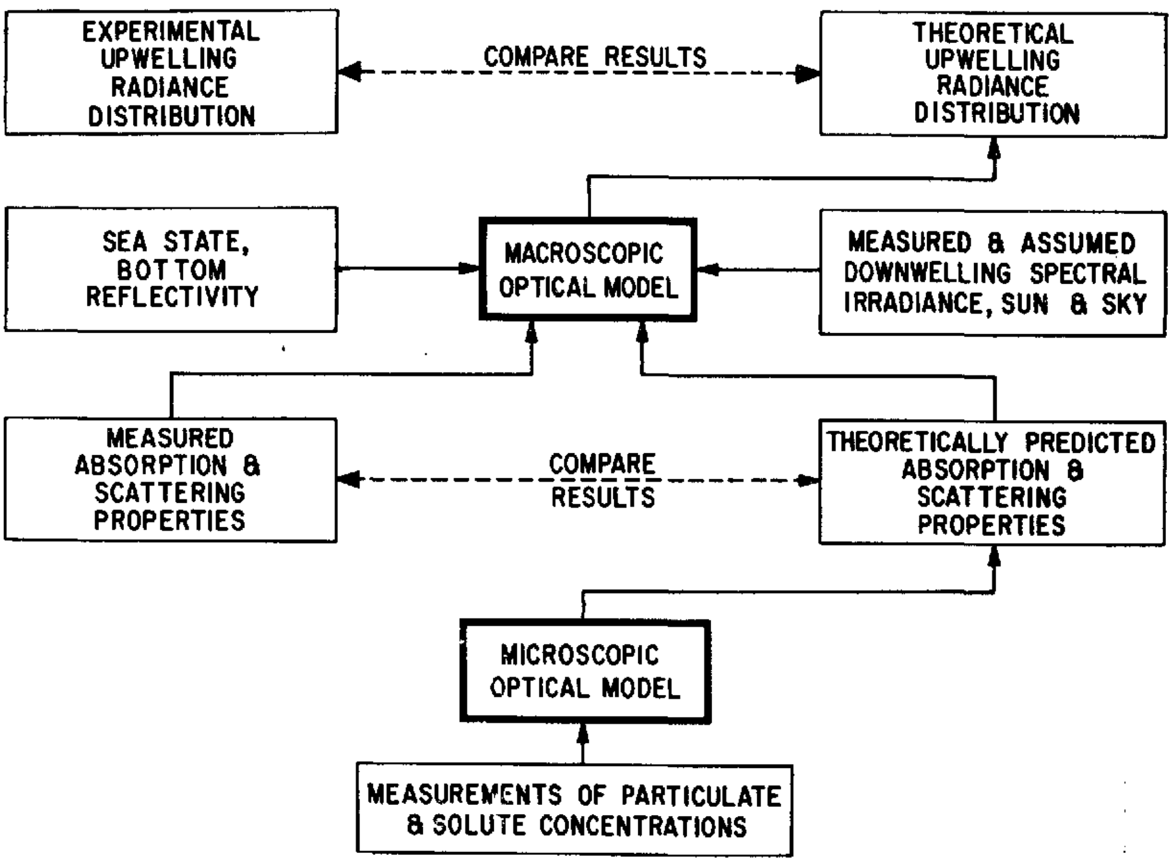


Figure 1. Optical Model of the Sea for Remote Sensing Applications

Molecular sizes in seawater (of optical importance) are considerably smaller than the wavelengths of visible light. Thus, the scattering properties of these constituents can be obtained theoretically using the theory developed by Rayleigh in 1871 and applied to liquids in 1910 by A. Einstein.[1]

The suspended particles, on the other hand, are comparable to and much larger than the wavelength of light so that Rayleigh's theory will be inadequate to treat the scattering produced by these particles.

In 1890 L. V. Lorenz[2] published the solution to the general problem of reflection and refraction of light by a transparent sphere. The origin of the theory has been widely attributed to a paper by Mie[3] in 1908 and the theory bears his name instead of that of Lorenz.

Although derived for a single sphere, the solution applies to any number of spheres, provided that they are all homogeneous in index of refraction, are randomly distributed in space, and are separated from each other by distances large compared with the wavelength.

In this case the total scattered energy will be equal to the algebraic sum of the contributions of scattered energy from all spheres in the scattering volume.

This approach appears to work quite well in atmospheric optics, where the spherical assumption is often valid and the Lorenz-Mie theory is directly applicable. In the sea, however, the particulates of major importance in the scattering process are in general highly irregular and the spherical assumption is no-longer valid.

Although the Lorenz-Mie theory has been shown to be experimentally valid for predicting the scattering by man-made <u>spherical</u> latex particles suspended in water[4], it is applicable to the highly irregular, <u>nonspherical</u> particulates (both organic and inorganic) suspended in seawater only at angles smaller than a few degrees.[5]

Thus a theoretical approach must be developed which is capable of accurately predicting volume scattering functions for polydisperse collections of the randomly oriented irregular particles found in natural waters. Once this technique has been developed, a full-scale computer simulation of the absorption and scattering properties of sea water can be set up using known and measured absorption data for water and the substances dissolved in it, using Rayleigh theory for scattering by the molecular constituents, and using the aspherical particle scattering theory for scattering by the suspended particles in seawater.

## THE MACROSCOPIC OPTICAL MODEL

In the development of the macroscopic model we assume that the spectral extinction coefficient c ($\lambda$) (the sum of the spectral absorption coefficient a ($\lambda$) and the total scattering coefficient b ($\lambda$)) and the spectral volume scattering function* $\beta(\lambda, \theta)$ are known as functions of depth throughout the upper 100 meters of the sea. The downwelling spectral irradiances of sunlight and skylight incident on the sea are also assumed to be known (separately).

The aim of the macroscopic model is to take this data, apply one of a number of possible theoretical approaches to the multiple scattering problem, and predict the upwelling spectral distribution of radiance emerging from the sea, assuming a perfectly flat, smooth sea surface and an infinitely deep ocean. Once this has been completed, a more realistic, rough upper surface and a shallow, reflective bottom can be added to the model.

## MULTIPLE SCATTERING THEORY

The propagation of radiation in an absorbing and scattering (but non-emitting) medium is governed by the equation of transfer for radiance in the following form:

$$\hat{\xi} \cdot \vec{\nabla} N(\lambda, \hat{\xi}, \vec{r}) = -c(\vec{r}, \lambda) N(\lambda, \hat{\xi}, \vec{r}) + N_*(\hat{\xi}, \vec{r}, \lambda)$$

where

$$N_*(\hat{\xi}, \vec{r}, \lambda) = \int_{4\pi} N(\hat{\xi}', \vec{r}) \, \beta(\hat{\xi}, \hat{\xi}', \vec{r}) \, d\Omega(\hat{\xi}').$$

In the above equation, $\hat{\xi}$ is a unit vector pointing at some arbitrary direction at a point in the medium specified by the position vector $\vec{r}$, $N(\lambda, \hat{\xi}, \vec{r})$ is the spectral radiance of the radiant field at the point $\vec{r}$, in the direction $\hat{\xi}$, and at the wavelength $\lambda$, $c(\vec{r}, \lambda)$ is spectral extinction coefficient at the point $\vec{r}$ and wavelength $\lambda$, $\beta(\hat{\xi}, \hat{\xi}', \vec{r})$ is the volume scattering function at the point $\vec{r}$ for light incident from the direction $\hat{\xi}'$ and scattered in the direction $\hat{\xi}$, and $d\Omega(\hat{\xi}')$ is an element of solid angle in the direction $\hat{\xi}'$. The equation of transfer

*The Volume Scattering Function (VSF or $\beta(\theta, \lambda)$) is defined by the following relationship:

$$\text{VSF} = \beta(\theta, \lambda) = \frac{1}{H_0(\lambda)} \frac{dI(\lambda, \theta)}{dV}$$

Where $H_0(\lambda)$ is the incident beam spectral irradiance and $dI(\lambda, \theta)$ is the element of light intensity in watts $\text{ster}^{-1}\text{nm}^{-1}$ scattered at angle $\theta$ from the element of scattering volume dV.

is a Fredholm integro-differential equation of the second kind and has no known general solution. Solutions are relatively difficult to obtain even in the most trivial cases. Most functional solutions are approximations and involve rather severe simplifying assumptions.

The main analytical approaches to solution and the various special formulations derivable from the equation of transfer are:

1. Invariant imbedding formulations (functional algebra and analysis).

2. Iterative procedures.

3. Monte-Carlo methods.

4. Spherical Harmonic methods.

5. Operator techniques (based on Fourier and Laplace transforms).

6. Diffusion equation approaches.

7. Special differential and integral models.

8. Perturbation techniques.

A description and critique of each of these may be found in Reference 6.

Most of the above approaches are not capable of handling the strongly asymmetric scattering functions exhibited by natural waters. (These functions are strongly peaked in the forward direction.) Other approaches are not suited for the arbitrary scattering functions which will be encountered and may also be discarded.

Of the remaining approaches, the Monte-Carlo technique appears to be the most promising for the following reasons:

a. The analytical tools needed for the Monte Carlo approach are relatively simple and easy to use, making implementation relatively straightforward and therefore not time-consuming.

b. The Monte-Carlo approach is flexible and can be used for a wide variety of experimental circumstances with very little modifications required for making changes.

c. The technique exhibits the fundamental physical processes in such a way that interpretation of the results in terms of those processes is not difficult.

d. The successful use of the Monte-Carlo approach in similar applications has already been demonstrated. [7,8,9]

The one major disadvantage of Monte-Carlo techniques (which is shared by many of the other techniques) is that even with currently available large and fast computers, the computation time can be quite high, especially when the calculations must be performed separately for a large number of different wavelengths (as is the case here).

Although a number of variance reduction techniques can be used to decrease the computation time required for a given accuracy,[10] they are not always as successful as one might like. C. Whitney has developed an alternative to the Monte Carlo technique[8] which appears to produce substantial savings in computation time over Monte Carlo methods.

Using one of these techniques, the macroscopic model should be set up for rapid, efficient calculations of the upwelling spectral radiance emerging from the sea for a large number of wavelengths throughout the visible portion of the spectrum based upon either measured or calculated input data, as shown in Figure 1.

## MEASUREMENTS OF SUBSURFACE OCEANOGRAPHIC PARAMETERS

There are a number of measurements which need to be made as a function of depth at several different coastal and offshore locations. These measurements will be needed for two different reasons, and therefore fall into two different categories.

First there are the measurements which are needed to obtain input data for the microscopic theoretical model. The data needed for this model are:

1. Concentrations and absorption coefficients of dissolved substances of optical importance.

2. Particle size distributions of each class of suspended particles which is known or expected to have a characteristically different index of refraction.

The second class of measurements that will need to be made are measurements of the particulate content of sea water using techniques which are more widely used and understood by oceanographers. These techniques include filtering and weighing (with several different methods of processing the filtrate both physically and chemically) and counting by optical and electron microscopy. These measurements are needed for correlation with the particle size analyses made using other methods and for correlation with both the observed and theoretically predicted upwelling spectral radiances.

## MEASUREMENTS OF BULK ABSORPTION AND SCATTERING PROPERTIES

In order to verify the predictions of the microscopic model and to provide accurate input data for the macroscopic model, measurements should be made of the bulk absorption and scattering properties as functions of both depth and wavelength at the selected locations. This will require the development of new instrumentation in order to make these measurements rapidly and accurately at various depths in the sea.

Actually, as discussed earlier, the absorption properties do not have to be measured directly but can be deduced from measurements of the extinction coefficient c and the scattering function $\beta$ over the full angular range of scattering.

The specialized instrumentation mentioned above would measure the extinction coefficient c and the volume scattering function $\beta$ at a number of fixed angles of scattering, both over the full spectral range of visible light (including extension into the near UV and near IR as far as is practicable).

## MEASUREMENTS OF THE UP- AND DOWN-WELLING LIGHT FIELD

In order to verify the predictions of the macroscopic optical model and to provide data for use with existing atmospheric optical models, the downwelling sunlight and skylight spectral irradiance just above the surface should be measured over the visible spectrum. In addition, the upwelling spectral radiance just below the sea surface should be measured, also over the visible spectrum.

## TECHNIQUES FOR OCEAN COLOR DATA ANALYSIS

Once the microscopic and macroscopic optical models have been developed and verified, they can be combined together into one model relating subsurface oceanographic parameters to upwelling spectral radiances. This model can then be coupled with any of several possible atmospheric models to predict upwelling spectral radiances at aircraft and orbital altitudes.

Using this final model, and the data collected experimentally, techniques can be developed for analyzing remotely sensed ocean color data to determine subsurface oceanographic parameters.

One aspect of this work could be the determination of criteria to guide the development of pattern recognition techniques as applied to multispectral ocean color data.

The problem of developing accurate and useful recognition techniques is more difficult for oceanic than for terrestrial data. On land, many of the features which one would wish to recognize have relatively well-defined spectral signatures and are frequently separated spatially on the surface. This is not true for oceanographic parameters which have generally less well-defined spectral signatures and seldom have identifiable sharp spatial boundaries. Because of these difficulties, it is felt that a combined observational and theoretical program, such as that outlined in this paper, offers the best hope for developing the reliable and accurate data analysis techniques which will be needed in the interpretation of ocean color sensor output data.

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